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Stéphane Cordier, Stéphane Cordier, Simona Mancini

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A brief review on numerical methods for the collisions operators

S. Cordier[1] S. Mancini[2]

1: Laboratoire MAPMO, CNRS UMR 6628, Université d'Orléans, 45067 Orléans, France, *stephane.cordier@univ-orleans.fr*
2: Laboratoire Jacques-Louis Lions, CNRS UMR 7598, Université Pierre et Marie Curie, BP 187, 4 pl. Jussieu, 75252 Paris, France, *simona.mancini@math.jussieu.fr*

1 Introduction

The evolution of a system of particles may be described at a microscopic level (particle description) or at a macroscopic one (hydrodynamic models). Kinetic models stand in between this two descriptions and are usually called mesoscopic models. They are used to describe the evolution of a great number of particles which are too many to be considered individually and are not in thermodynamic equilibrium, see [16, 17, 41]. In hydrodynamic models, the unknowns are macroscopic quantities like the particle density $\rho = \rho(x,t)$. On the other hand, in kinetic theory the unknown is the distribution function $f = f(x,v,t)$ representing the number of particles which at time $t > 0$ are in a position x with a velocity v, and satisfying a partial differential equation of the form:

$$\partial_t f + v\partial_x f + F\partial_v f = \tau^{-1} Q(f) \tag{1}$$

where τ is the relaxation time, i.e. the average time between two successive scattering events, F is the force field acting on the particles, and Q is the *collision* operator, describing the interaction of particles between them or with other particles present in the domain. We will see later on (Section 2) its many expressions. We just recall here that, in its more general form, Q acts only on the velocity v, and not on the position x. In many applications, the force field F is given in terms of external forces: gravitational, electric or crossed electro-magnetic forces; or it depends on the particles density, for example by means of the Poisson or Maxwell equations. In the remainder, we will focus on the numerical approximation of the right hand-side of equation (1), i.e. the collision part, refering the reader to [29] for what regards the left hand-side, i.e. the transport part.

The numerical approximation of kinetic equations is usually based on a time splitting (see [47]): one time step for the transport part and one for the collision one. More precisely, we consider equation (1) supplemented by the initial condition $f(x,v,t=0) = f_0(x,v)$. The solution after one time step Δt may be obtained by the sequence of two steps on the intervals $\Delta t/2$. First, we integrate the collision part: collision step. We remark, that in this case, the problem is space homogeneous, i.e. is independent with respect to the space variable x. Thus, we have for all x,

$$\partial_t \hat{f} = \tau^{-1} Q(\hat{f}) \ , \quad \hat{f}(x, v, 0) = f_0(x, v),$$

for a time step $\Delta t/2$. Then one approximates the transport part (convection step), using the result of the collision step as initial condition,

$$\partial_t f + v \partial_x f = 0 \ , \quad f(x, v, 0) = \hat{f}(x, v, \Delta t/2).$$

In other words, this splitting method uncouples the transport and collisions terms. It is proven to be convergent (see [43]) in some particular case. Moreover, in one time step Δt, we obtain an approximation of $f(x, v, \Delta t)$, and the process is iterated to obtain the numerical solution at later times.

We can discretize the collision part in many ways: discrete velocity methods, particle methods, finite volume, Monte Carlo or spectral methods. A survey of these different approximations will be given in Section 3. Let us remark that the time splitting scheme described above is first order accurate in space and time. Note that the order of accuracy of this splitting does not improve even if we solve with great accuracy both collision and convection steps.

In many engineering applications, the Euler or Navier-Stokes equations of fluid dynamics are not relevant and an accurate kinetic description through the Boltzmann equation of rarefied gas dynamics is required. From a computational point of view the numerical solution of the kinetic model is much more expensive than hydrodynamics one. This fact represents a real challenge for numerical methods, mainly due to the large number of variables in the problem and to the multi-dimensional nonlinear integral that defines the collision operator (see Section 2). Moreover, this integration has to be handled carefully since it is at the basis of the conservation properties of the Boltzmann equation.

The paper is organized as follows. In Section 2, we introduce the Boltzmann and Fokker-Planck operators describing the scattering of the particles, and some simplified versions like Lorentz, BGK and linearized models. In Section 3, we briefly describe the different numerical methods applied for the discretization of the collision operators. Section 4 is devoted to the presentation of the "Asymptotic Preserving Schemes". Finally, in Section 5 we present the numerical test which can be used to compare the various collision operators and approximation methods.

2 The collision operators

We introduce some operators which are more frequently used in the modeling of the particle collisions.

2.1 Boltzmann

The Boltzmann operator (derived in 1872) is a nonlinear, integral operator of the form:

$$Q_B(f,f)((v) = \int_{v_*} \int_{\omega \in S^2} B(f(v)\, f(v') - f(v_*)\, f(v'_*)\,)\, dv_*\, d\omega \qquad (2)$$

where the scattering cross section $B = B(|v - v_*|, \theta)$ represents the rate of particles which are scattered by the collision event from the velocities v and v' to the velocities v_* and v'_* respectively. We will call *target particles* those which are identified by the distribution function f_* and f'_*. In (2), we denote by ω the velocity angle, i.e. $v = |v|\omega$ with $\omega \in S^2$, and we call *deviation angle* the angle θ between the two relative velocities $|v - v_*|$ and $|v' - v'_*|$. Moreover, we recall a possible parameterization of the velocities after the scattering event (see [16]):

$$v' = \frac{v + v_*}{2} + |v - v_*|\omega\ , \quad v'_* = \frac{v + v_*}{2} - |v - v_*|\omega.$$

The scattering cross section B is usually determined by the type of interaction that the particles undergo. We refer to [56] for a review about the recent results in the mathematics theory of such collision operators.

2.2 Fokker-Planck-Landau

The scattering cross section B depends on the deviation angle θ, and on a small parameter ε, when taking into account also small deviation. For example in the Coulomb interaction case $B = B^\varepsilon$ is defined by:

$$B^\varepsilon = \sigma(\theta)\ \left(\log \frac{1}{\sin(\varepsilon/2)}\right)^{-1}\ \frac{\sin(\theta)}{[\sin(\theta/2)]^4}\ \chi_{[\varepsilon,\pi]}(\theta),$$

When $\varepsilon \to 0$, collisions become *grazing*, i.e. the scattering cross section concentrates at $\theta = 0$, and the Boltzmann operator converges to the nonlinear partial integro-differential Fokker-Planck-Landau operator (see [22, 25, 26, 34]):

$$Q_{FP}(f,f,)(v) = \nabla_v \cdot \left[\int_{v_*} \Phi(v - v_*)(\nabla_v f\, f_* - \nabla_{v_*} f_*\, f)\, dv_*\right], \qquad (3)$$

where $\Phi(z) = \|z\|^\gamma(\|z\|^2 Id - z \otimes z)$, and γ is related to the interaction potential. The more relevant case (from a physical point of view) corresponds to $\gamma = -3$, which is the Coulomb case.

2.3 Lorentz models

We now introduce the simplified versions of the Boltzmann and Fokker-Planck-Landau operators, known also as the Lorentz models, see [38]. Let us consider two species of particles of masses m_α and m_β such that: $m_\alpha \ll m_\beta$, for instance they can be electrons and atoms. Then, the distribution function of the light particles f^α must satisfy the following kinetic equation:

$$\partial_t f^\alpha + v\partial f^\alpha = Q(f^\alpha, f^\alpha) + Q(f^\alpha, f^\beta)$$

Developing in terms of m_α/m_β the collision operator $Q(f^\alpha, f^\beta)$, and passing to the limit $m_\alpha/m_\beta \to 0$, one gets that, at the leading order, the collision operator is independent with respect to the modulo $|v|$, see [24]. More precisely, $|v|$ appears in the first term of the above expansion only as a parameter, and the only variable changed by the scattering event is the velocity direction ω. This fact, is translated in the physical property that collisions are *elastic* (or equivalently that the target particles are immobile), and it holds both for the Boltzmann and the FPL operators. Their respective limits are the so called Boltzmann-Lorentz operator

$$Q_{BL}(f)(\omega) = \int_{S^2} B(|\omega - \omega'|)\,(f(\omega') - f(\omega))\,d\omega', \tag{4}$$

and the Fokker-Planck-Lorentz operator

$$Q_{LB}(f) = \Delta_\omega f(\omega), \tag{5}$$

also known as the Laplace-Beltrami operator. A numerical validation and a mathematical justification of this asymptotic may be found in [13, 20, 39].

2.4 BGK and linearized operator

Other simplified models are widely used, for example the BGK model. It consists in a simple relaxation of the distribution f toward the local thermodynamic equilibrium or the Maxwellian M

$$Q(f) = \tau^{-1}(M - Id)f\,, \quad M(v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|u-v|^2}{2T}\right), \tag{6}$$

where ρ, u, T are the density, mean velocity and temperature of the gas. We refer to [1, 27, 42] for more details.

Other simplified models are the linearized Boltzmann equation which are used in semiconductor modeling. In such models the target particles are replaced by a Maxwellian. See [41] for more details about such models.

2.5 Properties of the collision operators

During the evolution process, the collision operators (Boltzmann, FPL and BGK) preserve mass, momentum and energy:

$$\int_{\mathbb{R}^3} Q(f,f)\phi(v)\,dv = 0, \quad \phi(v) = \begin{pmatrix} 1 \\ v \\ v^2 \end{pmatrix}$$

and they satisfy the H-theorem, which express the entropy decay:

$$H = \int_{\mathbb{R}^3} f \log(f)\, dv\,, \quad \frac{dH}{dt} = \int_{\mathbb{R}^3} Q(f,f)\log(f) dv \leq 0.$$

The H-theorem implies that any equilibrium distribution function, i.e. any function f for which $Q(f,f) = 0$, has the form of a local Maxwellian distribution M.

We remark that, as the relaxation time $\tau \to 0$ in (1), the distribution function f approaches the local Maxwellian M defined by (6) and its moments (ρ, u, T) solve the Euler equations of gas dynamics, see [16].

3 Numerical methods

The main numerical methods usually applied in kinetic theory are: the discrete velocity method (DVM), the spectral method (SP) and the Monte Carlo method (MC). These methods correspond to different ways of representing the distribution function f.

3.1 Discrete velocity method

In the DVM the distribution function f is discretized and known on a fixed Cartesian mesh: $f_i(v,t) = f(v_i,t)$ for $i \in \mathbb{Z}^3$. The approximation of the Boltzmann equation by means of such methods begins with the works [8, 55].

The difficulty with this method is that quadrature formulae of the collision sphere are not well adapted with Cartesian grids. In fact, the consistency of these methods relies on the uniformity of repartition of Cartesian grid points on a sphere that can be related to problems in number theory. The discretized operator can be written as a sum of systems that involve admissible (i.e. cospherical) quadruples of velocities:

$$\frac{df_i}{dt} = \sum_{(i,j,k,l)\in A} B_{ij}^{kl}(f_k f_l - f_i f_j),$$

where A is the set of (triple)indexes of cospherical velocities and B_{ij}^{kl} are approximated values of the scattering cross sections. Once this system is splitted (known as 4-velocities or Broadwell models), it can be solved analytically. The main advantage in these methods is that each of this 4-velocities model can be interpreted as a model of admissible microscopic collision. Therefore, by construction, it is conservative and entropy decaying.

A series of paper have been written to obtain such numerical discretization for the FPL equation [11, 9, 10, 23, 37, 52], for BGK models [42] and for Lorentz models [20, 39].

Let us emphasize that these methods permit to obtain conservative and entropy schemes, i.e. the properties which insures the large time behaviour of the approximated solution as explained later on. Finally, we suggest a forthcoming book [3] which presents the state of the art in DVM approximations.

3.2 Spectral methods

The SP method has been recently proposed in order to approximate Boltzmann [49] and Fokker-Planck-Landau [50] operators. We briefly describe the idea of the method and refer to previous references for more details. Consider the FPL operator defined in (3). For simplicity, we assume that the support of the distribution function is included in the ball $B(0, R/2)$, $R > 0$. Next we approximate the distribution by a partial sum of a Fourier series,

$$f_N(t, v) = \sum_{k \in [-n,..,n]^3} \hat{f}_k(t) e^{i \frac{\pi}{R} k.v},$$

where $k=(k_1, k_2, k_3)$, n the number of half modes in each direction, and $\hat{f}_k$ is the $k-$th Fourier mode, see [12]. Considering the approximation $f_N(t, v)$, the collision part of (1), with collision operator (3), reduces to a differential system the form:

$$\frac{d\hat{f}_k}{dt} = \Big[\frac{\pi}{R}\Big]^{\gamma+3} \sum_{\substack{l,m \in (-n,..,n]^3 \\ l+m=k}} \hat{f}_l \, \hat{f}_m \Big[\hat{B}(l, m) - \hat{B}(m, m)\Big],$$

where $\hat{B}(l, m)$ is computed once for all using a recursive quadrature formula. In other words, SP method amounts to approximate the Fourier coefficient $\hat{B}(l, m)$ and to compute several sums of discrete convolutions. This can be done using a $n^3 \, log \, n$ algorithm based on a Fast Fourier Transform.

The SP approximation preserves mass, whereas variations of momentum and energy are controlled by the spectral accuracy. On the other hand, no information is available on the equilibrium states, the entropy decay and the positivity. One of the main advantage of the SP methods relies on the fact that both Boltzmann and FPL equation can be treated within the same framework (or numerical codes). The only difference being in the evaluation of the coefficient, since the structure of the differential system is unchanged.

3.3 Monte Carlo method

The most commonly used method is probably the MC method. It is based on a particle description of the distribution function, see [46], $f = \sum \delta_{(x-x_i) \otimes (v-v_j)}$, and on stochastic methods to evaluate the collision integral. We note that in this case, the transport part is solved exactly by moving the particle according to their velocity, see [29].

Pioneers of these methods are the direct simulation Monte Carlo method (DSMC), see [4, 5] and later the modified DSMC method, see [45]. Also, some convergence results are available in [2]. Finally, we refer to [47] for a recent presentation of these methods.

The common feature of these methods is to perform collisions between randomly chosen particles. These methods are not suitable for highly collision

regions since DSMC methods require a huge number of collision (i.e. they are too expensive).

Recently a different approach is proposed, with the goal of constructing simple and efficient numerical methods for the solution of the Boltzmann equation in regions with a large variation in the collision time τ, [15, 32, 48, 51]. These algorithms, called time relaxed Monte Carlo (TRMC) methods consists in projecting the solution towards the local Maxwellian for $\tau \ll 1$.

4 Asymptotic preserving schemes

As announced, a relevant situation where all the above methods lose their effectiveness is when considering flows where the collision time τ (equivalently the mean free path or the Knudsen number) varies over several orders of magnitude. In this situation there exists some highly collisional regions and others which are almost free-transport regions. Domain decomposition methods have been proposed for this problem. In these methods the computational domain is divided into a *fluid region* in which the system is treated by hydrodynamic equations as the Euler system, and a *kinetic region*, where the Boltzmann equation is used. Suitable matching conditions are then used to couple the two regions [7, 21, 40]. The main difficulties of this approach is the detection of the two regions and the description of boundary conditions at their interfaces.

Another alternative to deal with this difficulty is to use the "Asymptotic preserving schemes" (APS), i.e. compatible approximations with the large time behaviour. There are a lot of work that attend this difficulty. Let us mention, for instance, neutron transport or radiative transfer in the so called optically thick limit [36], Lorentz type operators [14] or the semi-conductors modeling [31, 35]. Let us also quote related papers for hyperbolic system with stiff source terms [18, 30, 33, 44]. Indeed, once discretized in velocities (using DVM), the kinetic models can be seen as a linear system of transport equations. This also is linked to the works on kinetic schemes for hyperbolic systems [54]: one replace the hydrodynamic system of interest by a kinetic formulation (usually of BGK type) in the $\tau \ll 1$ limit, i.e. the collision step reduces to the projection on the Maxwellian with the same moments. APS can be interpreted as a sort of kinetic scheme for the underlying Euler equations of gas dynamics [21].

5 Numerical test and conclusion

We refer to [12] for a comparison of the computational efficiency of DVM and SP methods. The proposed bench marks are homogeneous (exact solution, isotropic case, relaxation of temperature) and in non homogeneous

(Riemann problem with a finite Knudsen number or two interacting streams of particles).

The coupling with the transport part, to treat non-homogeneous situation, creates oscillations or discontinuities in velocity space and the treatment of the collision operator by fast algorithms becomes more complex, then it is necessary to use a robust method to obtain an accurate description of the distribution function. In [12], the Vlasov equation is solved by a high order semi-Lagrangian scheme preserving mass, impulsion, energy and positiveness (see also [29] for a review of the numerical treatment of the transport part). See also [28] for a comparison between MC and spectral method for the Boltzmann operator.

Let us also mention the focalization test [19] that can serve to determine whether or not a given collision operator have smoothing properties (like the FPL operator) or not (like the propagation of singularities with the Boltzmann equation as proved in [6])

A more complete description of the various models (Section 2), the various numerical methods (Section 3) and the numerical test (either in the homogeneous or the non-homogeneous cases) is needed to compare the approaches from the point of view of computational efficiency or large time behaviour (based on the preserved physical properties which ensure the trend to thermodynamic equilibrium). The brifly presented APS are a very promising direction of research (see Section 4) for treating more realistic situations.

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